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IBIS

Quarterly Report

Analysis of Cost:
CVD Diamond Deposition and Finishing

Contract Number: N00014-93-C2044

IBIS Associates, Inc.
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4th Quarter 1993

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Executive Summary

IBIS Associates has updated its predictive spreadsheet models of the CVD diamond film finishing technologies, and has solicited expert review for the DC arcjet, microwave, and finishing models. This report presents the results obtained with the new models and revised sets of baseline inputs for diamond heat sink manufacture.

For this report and the results contained herein, it is assumed that the regressions which estimate CVD diamond removal rates for the CVD Diamond Finishing model closely predict the actual removal rates for the technologies studied and that the input values for variables such as machine capacity are physically achievable.

The CVD diamond planarizing method of excimer laser ablation has been analyzed, and expert review conducted. This finishing process is low cost ($220/wafer) in comparison to the technologies analyzed to date: lapping ($997/wafer), oxygen plasma etching ($1,254/wafer), and oxygen ion milling ($7,698/wafer). Only hot iron diffusion ($144/wafer) is cost competitive with laser ablation for the assumed baseline conditions. For the laser ablation technology, the significant cost factors are related to the equipment costs, comprised of equipment, tooling, and maintenance, which constitute 24.8%, 25.0% and 11.4% of the cost respectively. In the case study analysis, the requirements for the finishing technologies are the removal of 111 micrometers (μ) of diamond thickness and that the technology achieve thermal management surface roughness specifications which, according to experts, ranges from 0.1 μ to 1 μ in height variation.

The DC Arcjet Model, with the inclusion of the kinetic theory of DC arcjet deposition, and the Microwave Model were last changed and reported during the third quarter of 1993. Fourth quarter progress on both models involved expert review. According to the models, the key factors driving the cost of thermal management diamond produced by the DC arcjet technology are the gas temperature, the power of the reactor, and the substrate diameter; the key factor driving the cost of thermal management diamond produced by the microwave technology is the power of the reactor. The reactor power has strong influence on cost for both technologies because it affects the scale-up of both linear growth rate and product size.

Overall, the expert review has been favorable. At Westinghouse, the DC arcjet and microwave models both received positive comments, and suggestions for change were minimal although the model failed to predict Westinghouse's deposition rate accurately. At Case Western Reserve, where just the DC arcjet model was reviewed, the deposition theory was supported by Professor John Angus. The microwave model received approval and little suggestion for change at Wavemat. The laser ablation CVD diamond finishing model preliminary results were favorable to Rocketdyne and Lockheed, and nominal changes were recommended. Lastly, useful warnings of the accuracy of theoretical prediction were contributed by Assistant Professor Cappelli at Stanford.

To be investigated further are the relationships between diamond growth rate and process yield for both the DC arcjet and microwave technologies. It is expected that as the growth rate increases, the yield decreases; yet a specific relation between these factors is unknown. Similarly, the relationship between substrate diameter and yield requires further investigation, due to the known complications with the increase of this parameter. In addition, the modeling of the combustion flame technology is in progress, as is the modeling of the metal particle thinning finishing technology. Lastly, expert approval of the models, as well as application of the models in conjunction with ARPA-funded companies developing diamond technology (e.g. Norton, Astex), is continually in progress.

Modeling Progress

The seven steps for the fabrication of diamond film are Surface Preparation, Deposition, Etching, Laser Trimming, Lapping, Microscopic Inspection, and Thermal Conductivity Inspection. The flowchart for the process is shown in Figure 1, and descriptions for the processes can be obtained from previous quarterly reports.

The progress of the CVD diamond thin film models has involved both deposition improvements and the addition of the finishing operation of laser ablation. The changes to the deposition steps are described later in this report, and the laser ablation operation is described in the following section.

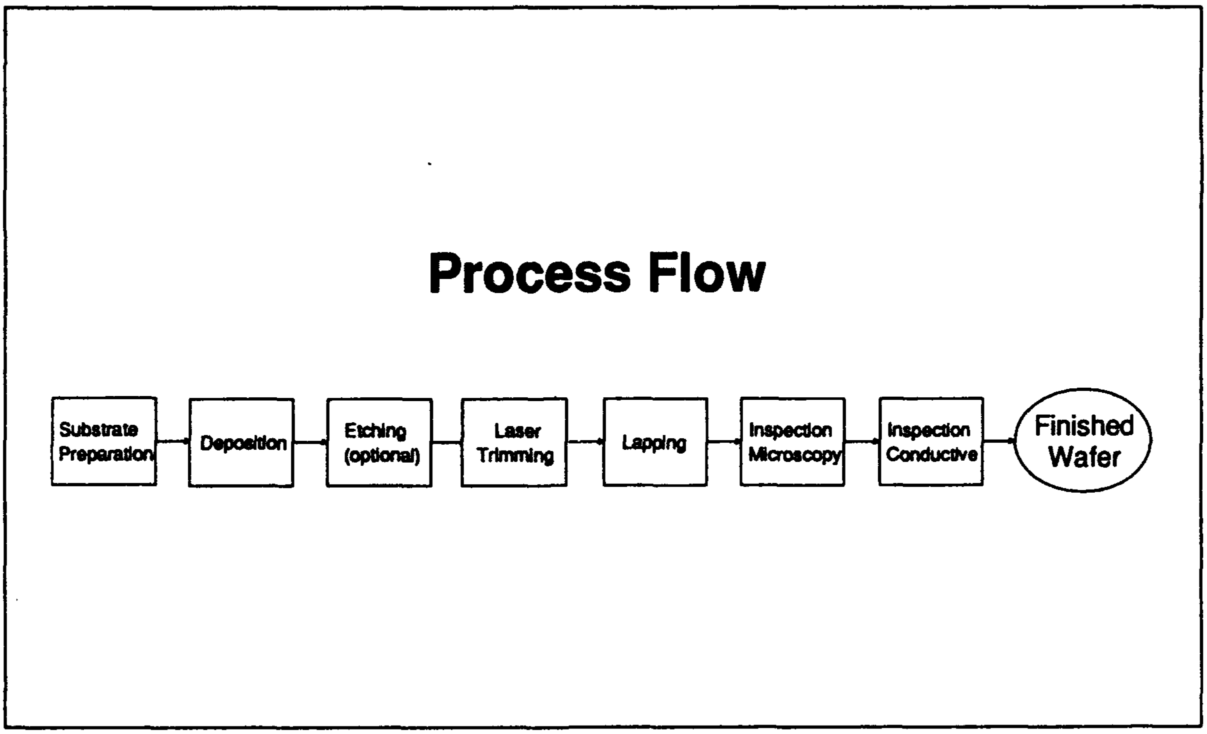

Figure 1

Excimer Laser Ablation

The deposition methods modeled by IBIS deposit polycrystalline diamond across the deposition area with micro- and macro-surface height variation. For thermal management applications in electronics, however, the surface of the diamond thin film must be planarized. Four technologies were analyzed for the second quarter report of 1993. The sensitivity analysis section compares the cost of the different technologies, which must remove roughly 100 μ of diamond thickness.

Approach

The rapid delivery of energy into a material will vaporize the region which absorbs this energy, assuming that the energy concentration is above the material's vaporization threshold. For the excimer laser ablation of diamond, energy pulses can be focused over areas ranging from one square micron to over one square centimeter. Depending on the energy and the area of these pulses, diamond will or will not be ablated. The energy per unit area, or fluence, is the process parameter which determines the occurrence and depth of the ablation. For a material at constant temperature, and a laser of constant wavelength, a relationship can be determined experimentally that correlates fluence to depth of ablation, or etch depth. Such relationships have been derived for diamond-like carbon and natural IIa diamond. Although it has not been identified through the public literature, a relationship for polycrystalline CVD diamond for thermal management applications should lie between the two existing plots, according to experts in laser ablation. Figure 2 shows these two curves, and the assumed relationship for thermal-grade polycrystalline CVD diamond.

Inputs

Model List 1 shows the inputs to the laser ablation operation. There are three unique input subsections that require a brief description: the power efficiency section, the beam characteristics section, and the tooling inputs section.

Two power efficiency inputs are used in the model to calculate the utility requirements of the laser ablation equipment. The model calculates the power imparted to the material at the input beam energy and frequency, then the machine power requirement is determined from the efficiencies in transforming electricity to laser energy and initial laser energy to delivered laser energy.

The important process parameters for the laser ablation finishing technology are the total pulse energy, laser frequency, and the beam area. These inputs, with the assumed relationship between etch depth and fluence, determine the diamond removal rate which drives the cost of the operation. The baseline model assumes mid-range values for these critical input parameters.

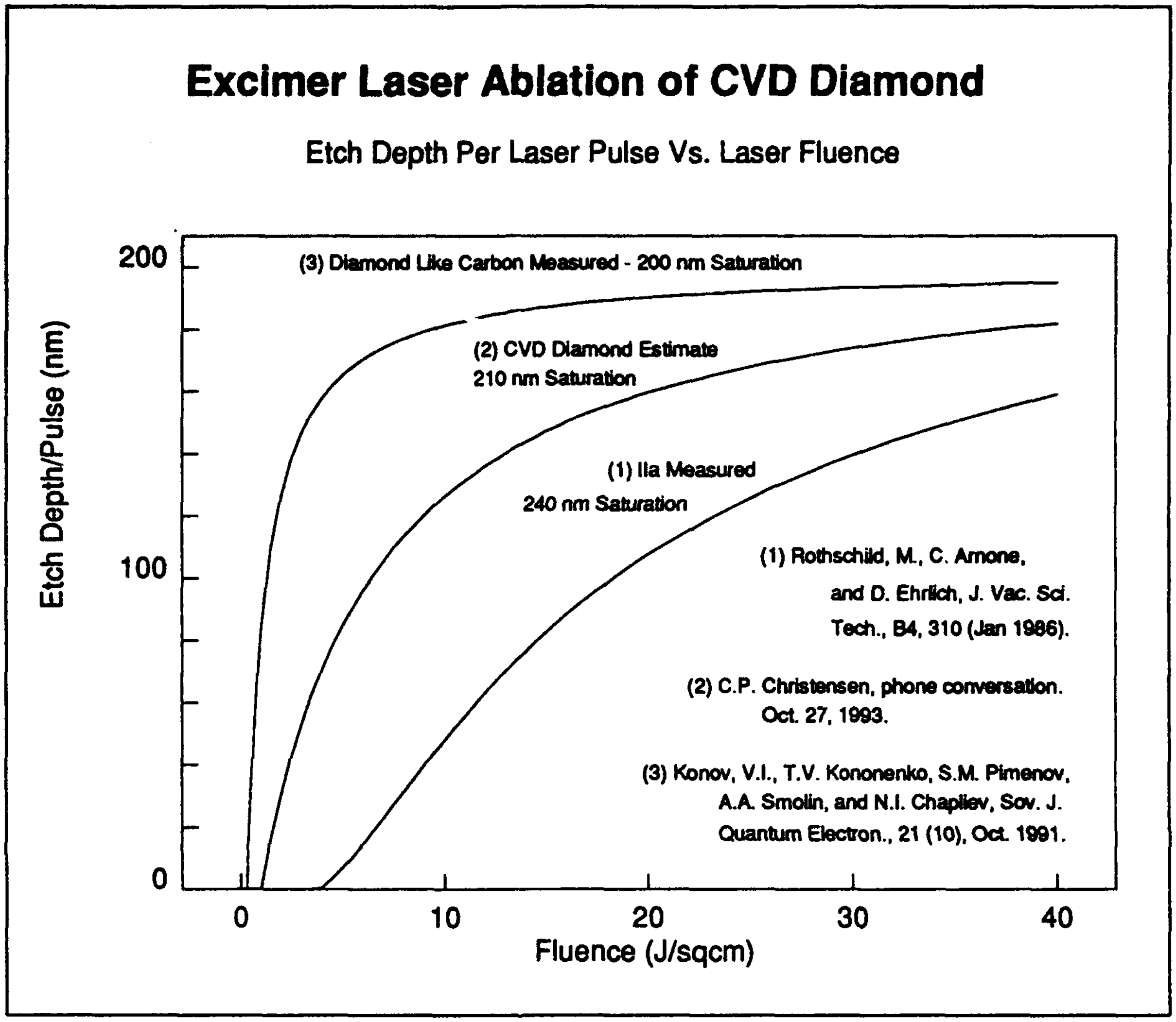

Figure 2

Lastly, the useful tool life and laser tool cost inputs determine the tooling costs for the operation. The electrode assembly, or vessel, is the tooling in an excimer laser generator that excites the lazing gases, and requires replacement after roughly one billion pulses. Industry experts suggest that the cost of replacement for this device ranges from ten to fifteen thousand dollars, depending on the power and supplier of the laser.

CVD Diamond Finishing: Laser Ablation Inputs

```
--------------------------------------------------------------------------
          CVD DIAMOND FINISHING TECHNICAL COST MODEL
          IBIS ASSOCIATES, INC.          Copyright (c) 1991 v4.0
--------------------------------------------------------------------------
                                         Revision Date: 12/13/93
PRODUCT SPECIFICATIONS
                   Part Name 6 in. substrate          NAME
              Wafer Diameter      15.24 cm            DIAM
    Finished Wafer Thickness      1,000 um            THIK

    Annual Production Volume          1 (000/yr)      NUM
    Length of Production Run          5 yrs           PLIFE

PROCESS RELATED FACTORS - EXCIMER LASER ABLATION
        Dedicated Investment       1.00 [1-Y 0-N]     DED9
               Process Yield      90.0%               YLD9
  Average Equipment Downtime      15.0%               DOWN9
   Direct Laborers Per Station     0.25               NLAB9

      Power:Laser Efficiency        1.0%              PLEFF9
     Laser:Optics Efficiency      75.0%               LOEFF9

          Total Pulse Energy     400.00 mJ            PENGY9
             Laser Frequency     200.00 Hz            FREQ9
             Total Beam Area      10.00 mm^2          NSPOT9

     Lasing Gases                  Menu #        vol%
     ------------------------------------------------
     KrF                             2         100.0% GAS9A VOL9A
     None                            0           0.0% GAS9B VOL9B
     None                            0           0.0% GAS9C VOL9C
     ------------------------------------------------
                                               100.0%

            Material Removed      10.0%by wgt         MREM9
 Load/Unload and Clean Wafers     30.00 min/batch     PTIME9
            Useful Tool Life   1.00E+09 pulses        LIFE9
             Laser Tool Cost    $12,500 /ea           TOOL9
  Laser XY Table, Optics Cost  $100,000 /sta          MCH9A
         Total Gas Flow Rate     100.00 sccm          TFLOW9

    Available Polishing Time      8,640 hrs/yr        DAYHR9
   Building Space Requirement       400 sqft/sta      FLR9
```

Model List 1

Excimer Laser Ablation Cost Estimates

Model List 2 shows the cost summary for the laser ablation of CVD diamond using the inputs from Model List 1. The cost of removing 111 µ thickness of diamond from a six inch diameter wafer costs $220 per wafer. This process is capital intensive, with equipment related costs (equipment 24.8%, tooling 25.0%, and maintenance 11.4%) at 61.2% of the total cost. As a capital intensive operation, laser ablation costs are highly sensitive to the assumptions of annual production volume and dedicated equipment. Second in significance are labor costs, at 21.4% for this finishing operation.

CVD Diamond Finishing: Laser Ablation Cost Summary

DIAMOND FINISHING: LASER ABLATION
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	per piece	per year	percent	investment
VARIABLE COST ELEMENTS				
Material Cost	$0.01	$11	0.0%	
Direct Labor Cost	$34.48	$34,482	15.7%	
Utility Cost	$2.14	$2,137	1.0%	
FIXED COST ELEMENTS				
Equipment Cost	$54.52	$54,523	24.8%	$272,616
Tooling Cost	$55.00	$55,000	25.0%	$275,000
Building Cost	$2.00	$2,000	0.9%	$40,000
Maintenance Cost	$25.01	$25,009	11.4%	
Overhead Labor Cost	$12.50	$12,500	5.7%	
Cost of Capital	$33.97	$33,971	15.5%	
TOTAL FABRICATION COST	$219.63	$219,634	100.0%	$587,616

Model List 2

It must be noted that these cost estimates incorporate three critical assumptions. First, it is assumed that the relationship between fluence and etch depth in Figure 2 is valid for thermal management CVD diamond. Second, the model assumes that the rate limit for this operation is the frequency of the laser. For this to be true, the laser must never pause to change locations on the CVD diamond workpiece. The last assumption involves yield. For this operation, yield is assumed to be 90%. In laser ablation, expected yield reductions would be due to defect propagation from thermal-induced mechanical cycling in addition to the creation of heat-affected zones, where mechanical strength is reduced and subsequent failure might occur. The effect of these phenomena on yield are not incorporated in the model.

Sensitivity Analysis

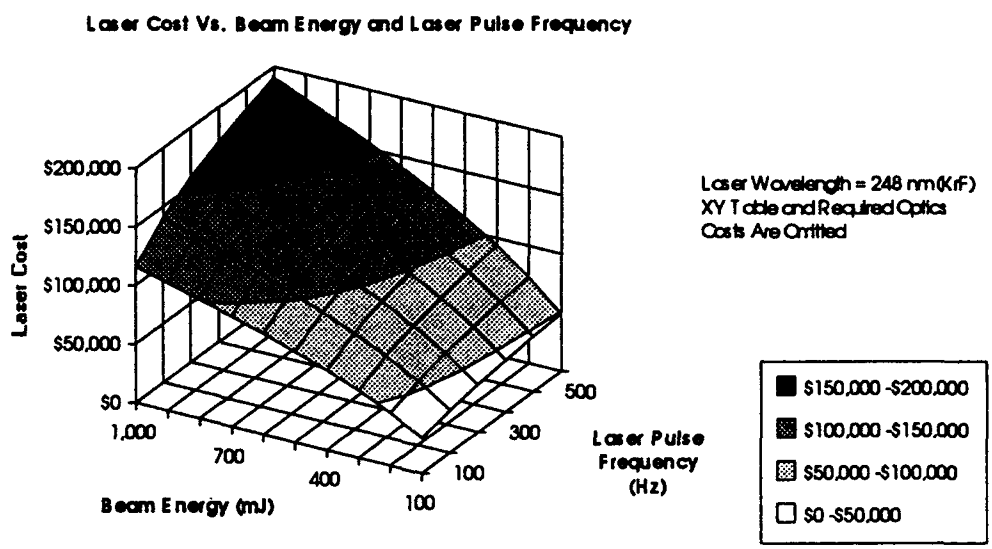
One of the advantages of a Technical Cost Model is that it permits the flexibility of performing sensitivity analyses. Using sensitivity analyses, it is possible to explore the cost implications of changing key input variables such as production volume, material prices, product dimensions, etc. As an R&D management tool, these analyses help set development goals for cost effective manufacturing. Further, they help in long term planning, by indicating the cost savings that may be realized through scale-up. Presented in the following sections are the following analyses:

- Machine Cost Vs. Beam Energy and Laser Frequency
- Etch Volume Per Pulse Vs. Beam Energy and Beam Area
- Cost Per Wafer Vs. Beam Energy and Beam Area

- Cost Per Wafer Vs. Beam Energy and Laser Frequency
- Cost Per Wafer Vs. Thickness Removal (All Technologies)

Machine Cost Vs. Beam Energy and Laser Frequency

From data collected on industrial excimer lasers, the price of a laser, excluding the computer driven XY table and associated optics, varies directly with the laser pulsing frequency and pulse energy but inversely with the wavelength. A regression equation was derived for the price of the laser, without peripheral equipment, as a function of these variables. This relationship is shown in Figure 3 for the wavelength of 248 nanometers. Figure 3 does not show the baseline optics and XY table price, which is assumed to be $100,000. For the model, a baseline beam energy of 400 mJ and frequency of 200 Hz was assumed, which correlates to a laser cost of $82,000.



Note: This cost estimation graph was generated after making numerous assumptions, which are detailed in this report.

Figure 3

Etch Volume Per Pulse Vs. Beam Energy and Beam Area

Based on the relationship shown in Figure 2, lasers of varying beam area and energy have optimal settings, as shown in Figure 4. It is assumed that the beam area can be changed by adjusting the existing optics, without affecting cost. For the baseline laser energy of 400 mJ, the optimal beam area is roughly ten square millimeters. Approximately 500,000 cubic microns are removed per laser pulse at this laser setting. At the input frequency of 200 Hz, 378 cubic millimeters of polycrystalline CVD diamond can be removed per hour, requiring over five hours to remove the baseline volume of two cubic centimeters.

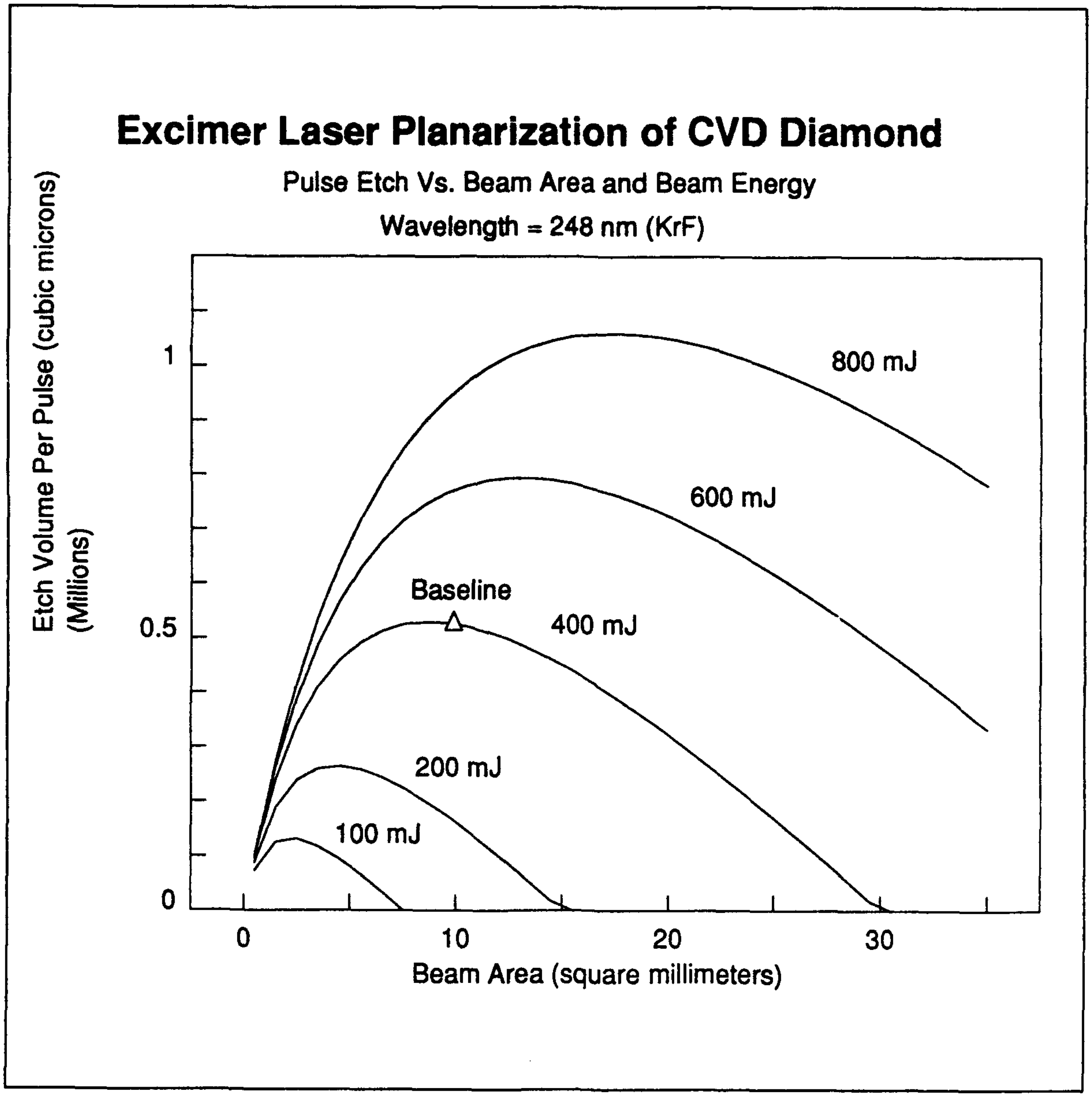
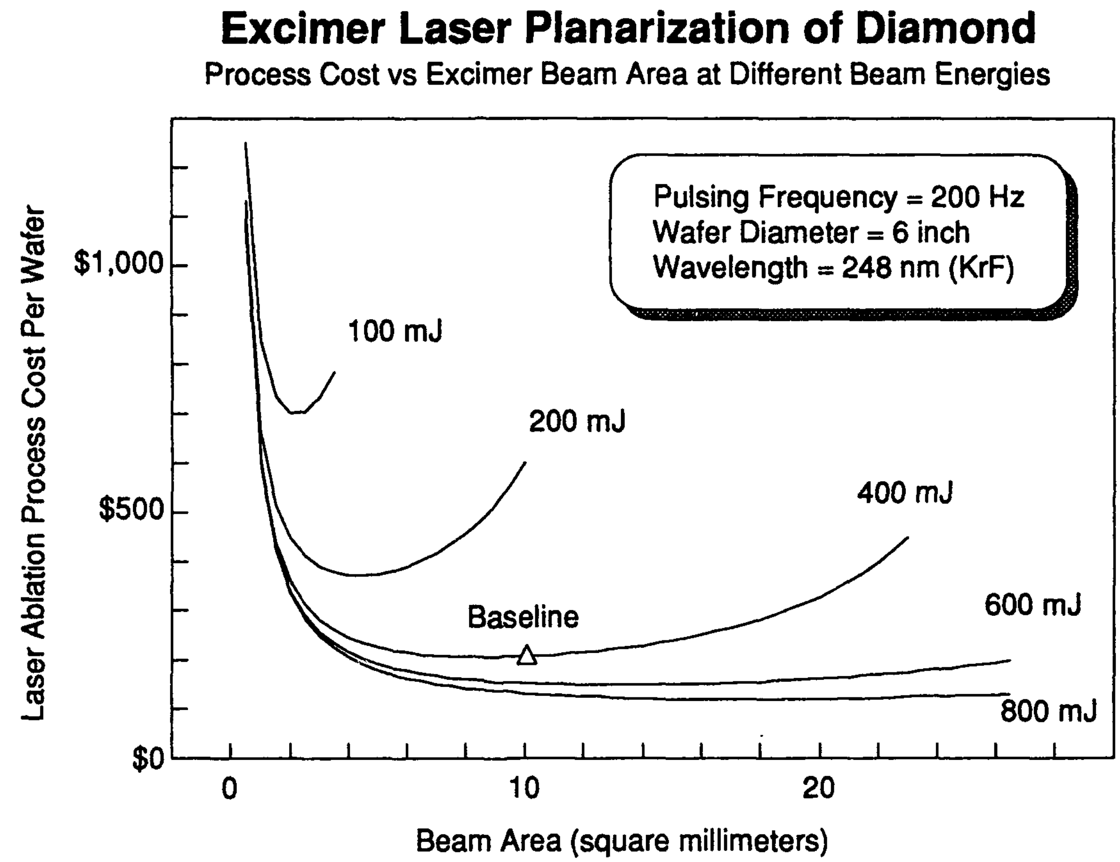


Figure 4

Cost Per Wafer Vs. Beam Energy and Beam Area

At these baseline laser settings, the cost per six inch wafer is $220. As shown in Figure 5, the optimal volume removal settings translate to optimal costs. The optimal cost for the laser ablation of the CVD polycrystalline diamond wafers ranges from $700 at 100 mJ and two square millimeters, to $120 at 800 mJ and eighteen square millimeters. It must be noted that these cost estimate curves are derived from assumptions which are described in the Approach section of this report, and include specifically the assumption of constant yield.



Note: This cost estimation graph was generated after making numerous assumptions, which are detailed in this report.

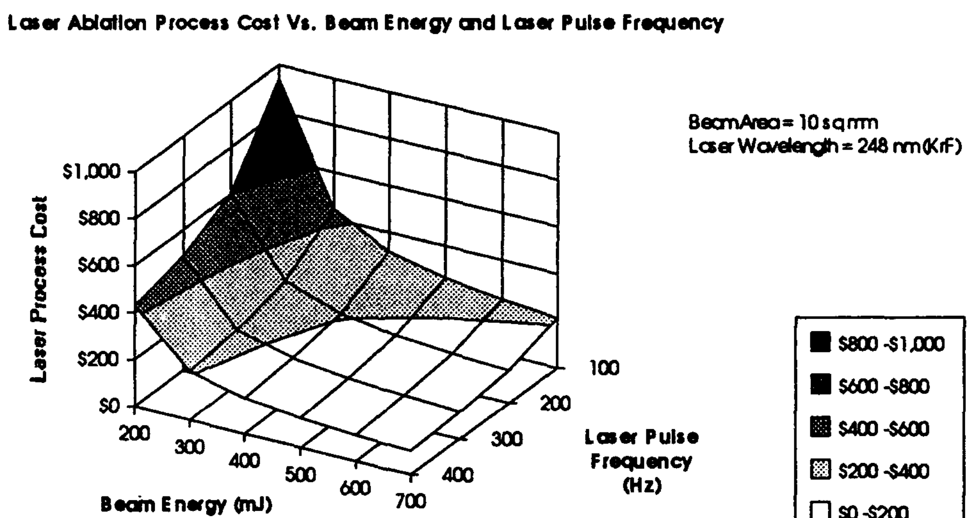
Figure 5

Cost Per Wafer Vs. Beam Energy and Laser Frequency

Figure 5 also shows the cost reduction with varying beam energy at constant area. Figure 6 illuminates the effect of beam energy further while showing the effect of laser frequency. At constant beam area, wafer dimensions, and material removal, the cost of finishing polycrystalline CVD diamond wafers can be approximated by the equation:

$$\text{Finishing Cost} = 10^{6.61} * (\text{Beam Energy})^{-1.14} * (\text{Laser Frequency})^{-0.55}. \qquad 1.$$

Therefore, a doubling of the beam energy results in a 55% reduction in cost while a doubling of the laser frequency decreases cost by 32%. It must be noted that this cost estimate curve is derived from assumptions which are described in the Approach section of this report.

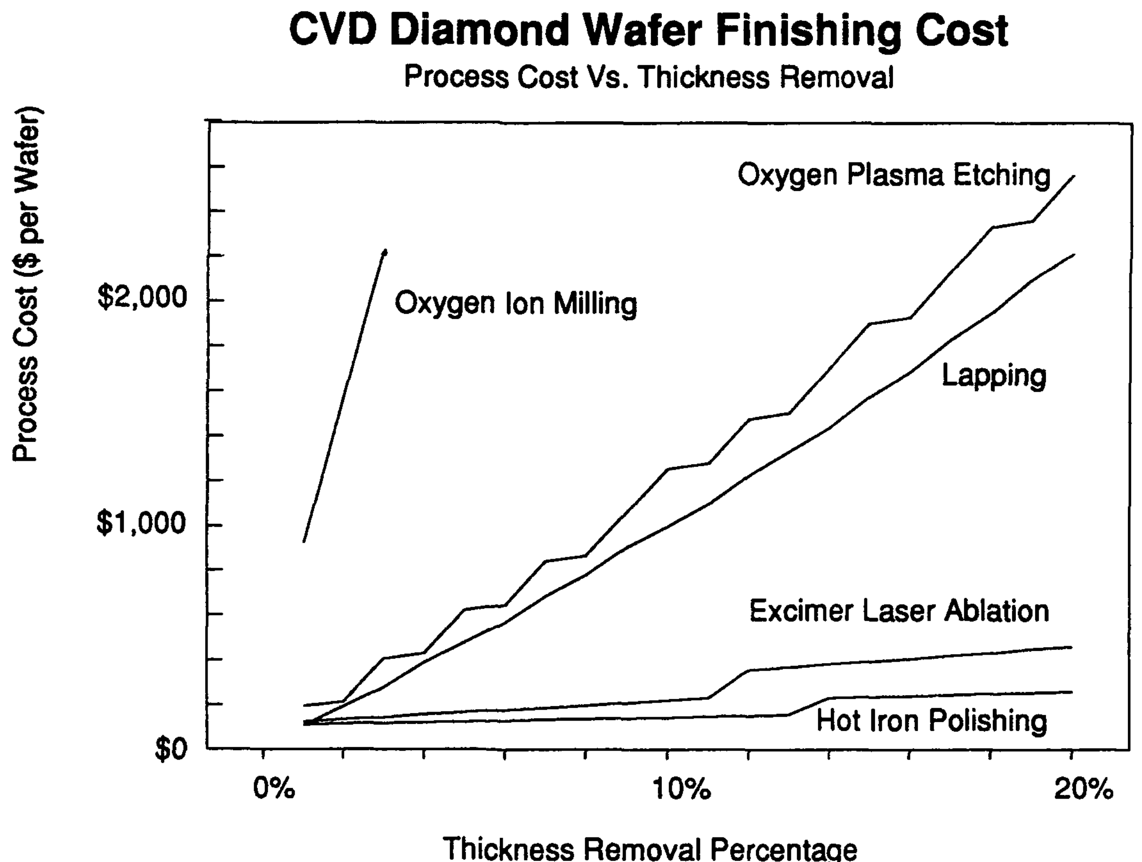


Note: This cost estimation graph was generated after making numerous assumptions, which are detailed in this report.

Figure 6

Cost Per Wafer Vs. Thickness Removal (All Technologies)

It is possible to evaluate the different polishing methods by comparing wafer cost to the weight percent of diamond that is removed. Figure 7 shows cost per wafer as a function of the deposited material removal percentage. In comparing finishing technologies, the best technique yields the final surface finish while removing diamond at a high rate. In Figure 7, this translates to flat or shallow sloped curves. Abrasive Lapping and Oxygen Plasma Etching, for small diamond removal, are relatively inexpensive. Lapping is competitive for low material removal percentages due to low capital costs, but increases quickly due to its slow removal rate. Alternatively, Oxygen Plasma Etching is competitive for low material removal percentages due to its high removal rate, but increases quickly due to its high capital costs. With higher removal rates, the Hot Iron Diffusion and Laser Ablation



Note: This cost estimation graph was generated after making numerous assumptions, which are detailed in this report.

Figure 7

operations remain relatively inexpensive with increasing mass removal percentages, and therefore have the shallower slopes. The step-like jumps in these graphs are due to increases in the number of duplicate polishing stations.

For these analyses, the yields are assumed to be unaffected by removal rates. Expert review has revealed that the yield of each finishing technology decreases as the removal rate increases. The expert review of this model is discussed in the Expert Review section of this report.

Future Work

There exist other finishing technologies that require cost modeling, as well as improving laser ablation to include YAG laser technology. Work on finishing for the first quarter of 1994 will include the modeling of the Power Metal Diffusion and possibly the SiOx technologies. Lastly, the technologies already modeled will be updated with new information.

DC Arcjet Model

The progress of the DC Arcjet Model, as stated above, has involved only the expert review of the model, which is described in the Expert Review section of this report. In addition, an in-depth explanation of the DC Arcjet deposition theory is provided in this report, describing the use of Professor David Goodwin's deposition theory in the model.

Scaling Laws for DC Arcjet CVD Diamond Deposition

The DC Arcjet Model is able to rapidly estimate the linear growth rate of diamond through the application of theoretical scaling laws developed by Professor David G. Goodwin at CalTech. These scaling laws combine models of atomic hydrogen transport and diamond surface chemistry to arrive at a prediction of growth rate.

The growth rate prediction section of the DC Arcjet Model and the scaling laws on which it is based make the following assumptions and simplifications.

- The feedstock gas is a dilute hydrocarbon in a carrier gas mix of H_2 and a non-reactive gas.
- The concentration of atomic hydrogen is defined by the thermally driven dissociation of molecular hydrogen and is assumed to be in equilibrium.
- The substrate temperature is near 1200 K.
- The effects of oxygen or halogens on diamond growth are not considered.
- Conditions are such that high-quality diamond is being grown.
- The incorporation of adsorbed hydrocarbons into the diamond lattice is assumed to be first-order.
- The etching of adsorbed hydrocarbons by atomic hydrogen attack is assumed to be first-order.
- Defects are generated when an adsorbed hydrocarbon reacts with a nearby adsorbed hydrocarbon before is is fully incorporated into the lattice.
- The rate of defect generation is proportional to the number of adsorbed hydrocarbon pairs on the surface.
- Adsorbed hydrocarbons are randomly distributed on the growth surface.
- Conditions are such that the region from the exit nozzle to the boundary layer is assumed to be isothermal, as shown in Figure 8.

The basic concept behind the scaling laws is that the growth rate of diamond is an exponential function of the concentration of atomic hydrogen at the substrate surface,

$$G \propto X_d [H]^n \qquad 2.$$

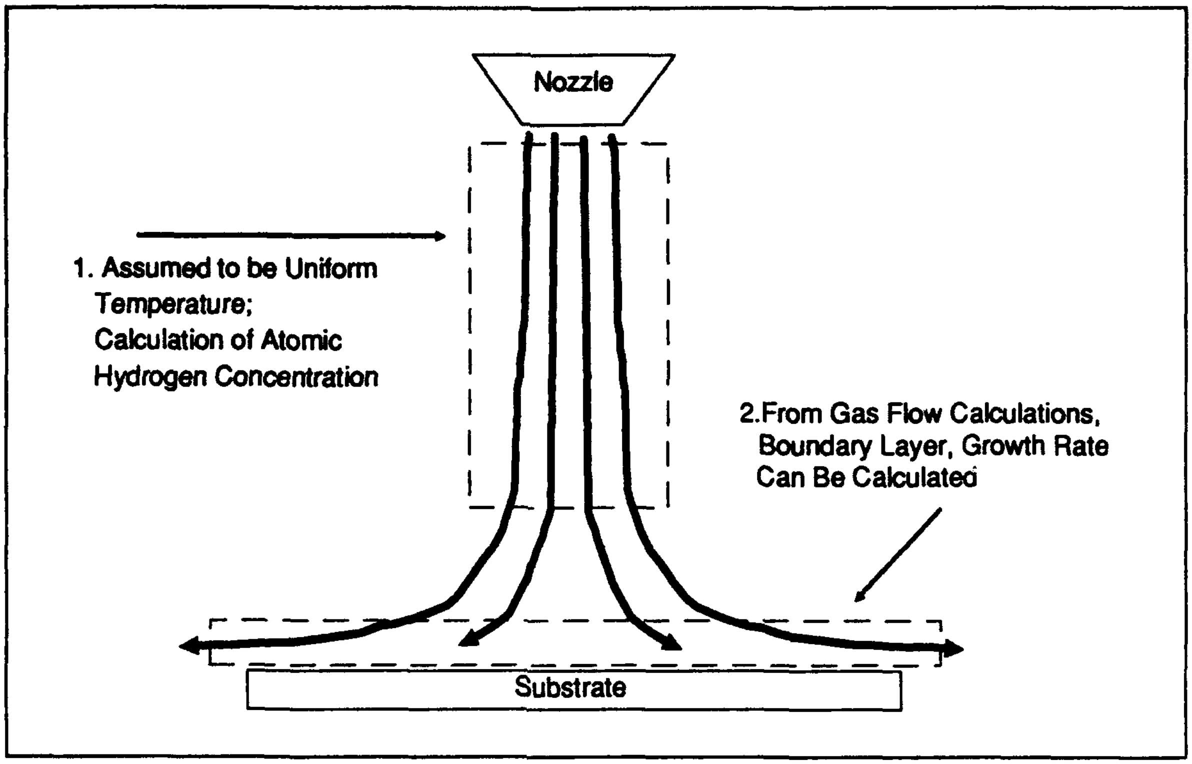


Figure 8

where "G" is the diamond linear growth rate, "X_d" is the defect density which is defined by desired diamond quality, "[H]" is the atomic hydrogen concentration at the substrate surface and "n" is some number between 1 and 2.

The steps used to predict the growth rate in the DC Arcjet Model are outlined in detail below.

1. The mole fractions of various gas species in the arcjet nozzle, far from the substrate, are calculated from the gas temperature, reaction energies and the NASA enthalpy constants. For instance, for atomic hydrogen, the following reaction and equilibrium computations are made:

$$H_2 \xrightarrow{k_p} 2\,H\cdot \qquad 3.$$

$$\text{where } k_p = \frac{[H\cdot]^2}{[H_2]} = e^{-\Delta G/RT} \qquad 4.$$

where ΔG, the free energy, of the reaction is computed from the NASA enthalpy constants.

2. The gas velocity far from the substrate is calculated based on gas flow rate, mass transfer theory, the duct area, the reactor pressure and the mean molecular, calculated from the mole fractions.
3. The specific heat ratio is calculated from the mole fractions and the specific heat of each gas species.
4. The speed of sound is calculated from the specific heat ratio, the gas temperature and the mean molecular weight.
5. The Mach number, the ratio of the speed of the gas flow to the speed of sound, is calculated from the gas velocity and the speed of sound.
6. The parameter "a", the radial velocity gradient just outside the boundary layer, is calculated from the Mach number.
7. The boundary layer thickness is calculated from the parameter "a".
8. The atomic hydrogen concentration at the substrate is calculated from the boundary layer thickness and transport considerations.
9. The growth rate is calculated using the atomic hydrogen concentration at the substrate based on Equation 1, and is calibrated using an actual data point relating to the production of thermal management quality diamond.

The scaling laws used in the DC Arcjet model are described in greater detail in D.G. Goodwin, "Scaling Laws for Diamond Chemical Vapor Deposition. I. Diamond Surface Chemistry," J. Appl. Phys. vol. 74, pp 6888-6894 and D. G. Goodwin, "Scaling Laws for Diamond Chemical Vapor Deposition. II. Atomic Hydrogen Transport," J. Appl. Phys. vol. 74, pp 6895-6906.

Future Work

Working towards a more powerful version of the DC Arcjet Model, a few goals remain. First, expert review is in progress and will continue for the duration of the project. Second, work remains in establishing correlations between growth rate and yield, and substrate diameter and yield.

Expert Review

The verification of a cost model with industry experts is critical to the model's evolution. During the fourth quarter of 1993, numerous meetings with CVD diamond authorities were conducted to provide criticism on the IBIS cost models. The centers of expertise that were visited include Case Western Reserve, Westinghouse, Wavemat, Rockwell's Rocketdyne division, Lockheed, and Stanford University.

Case Western Reserve - The John Angus Group

Professor Angus does not work with the DC arcjet technology, and therefore did not offer criticism about the geometric assumptions, but he did approve of Goodwin's work and seemed to agree with the chemical theory assumptions, with the criticism that the model should take into account the affects of acetylene concentration on the growth rate. As for the inverse relationship of growth rate with gas temperature to the fourteenth power, he felt that was too drastic. (Subsequent IBIS analysis has shown that this exponent is more likely about six.)

Westinghouse - DC Arcjet Model

Using the IBIS model with Westinghouse proprietary inputs, the model's predicted linear growth rate was off by roughly a factor of five; however, differences between the Westinghouse arcjet and other arcjet processes may explain this discrepancy. When discussing the model's use of the Goodwin deposition theory, their deposition theorist Dr. Robert Young agreed with Goodwin's assumptions for the DC arcjet theory. Westinghouse was interested in the model predictions for their higher power systems, and asked to have the printouts from this meeting.

Rocketdyne Division, Rockwell International

Rocketdyne had the following criticisms of the IBIS laser ablation work:

- The relationship between etch depth and fluence should be shifted upward. Specifically, there should be a higher etch depth per pulse. There was some confusion about their data to support this assertion, however, so future communication between IBIS and Rocketdyne will target the etch depth - fluence relationship.
- They agreed that the trend for this same relationship would saturate due to a gas plasma being created with higher fluences.
- Accuracy of laser ablation (+/- surface height error) is a function of focusing angle: the angle at which the light in the beam converges from the lens to its focal point is also the angle at which light energy diverges after the focal point. Consequently, high angle focusing results in more accurate laser ablation. This information allows us to conclude that beam depth accuracy is not necessarily a function of beam focal spot diameter.

Lockheed Missiles & Space Company, Inc.

At Lockheed, Dr. Ravi met with IBIS to discuss the combustion flame CVD diamond deposition technology and excimer laser ablation. An account of the combustion flame portion of the meeting will be provided along with the combustion flame results in the first quarter 1994 report. With respect to the excimer laser ablation of polycrystalline CVD diamond, Lockheed's experience has shown that the etch depth per laser pulse is a function of the temperature of the substrate.

Stanford University

At Stanford, Assistant Professor Mark Cappelli talked about his concerns with the accuracy of the IBIS cost estimates. According to Prof. Cappelli, theoretical models of deposition that have been developed do not predict accurately, but are modified for each new data point. While there is some truth to this statement, he was not convinced that David Goodwin's models are any more accurate than his own. Overall, the meeting was a useful warning for IBIS to be careful about the misleadingly simple presentation of cost, which is based on many assumptions.

Westinghouse - Microwave Model

Meeting with Dr. Young and Dr. Partlow, the linear growth rate prediction section of the TCM was discussed at length. Many of the assumptions and simplifications which are made in the model were identified, along with their consequences. Dr. Young contested the assumption made in the Goodwin model that there is a local thermal equilibrium in the gas; that is, that the gas can be assumed to be at a single temperature rather than trying to estimate the temperature of the electrons and each species present in the gas. He said that it is not well known how important this assumption may be when trying to estimate linear growth rates based on the Goodwin model.

After discussing the model, the model was used to predict the linear growth rate of one of the Westinghouse microwave reactors. Dr. Partlow provided the input parameters and the linear growth rate for a recent run. The IBIS TCM correctly predicted the linear growth rate to within 0.05 u/hr. Drs. Young and Partlow were both very impressed with the model's predictive abilities and asked to have a printout of the simulation of their reactor.

Wavemat

Meeting with Dr. Dahimene, the linear growth rate prediction section of the TCM was discussed at length. Many of the assumptions which are made in the model were identified, along with the consequences of these assumptions. Dr. Dahimene's main concern with the linear growth rate predictive model was the equation

$$\text{Linear Growth Rate} = Z * [H]_{(0)}^2. \qquad 5.$$

Dr. Dahimene was disappointed with this approach to growth rate prediction but was still curious as to how closely the model could predict rates based on data from one of Wavemat's reactors. Also, Dr. Dahimene was concerned that the reactor pressure did not enter into the growth rate calculation. He explained that there are several factors in the linear growth rate predictive model such as plasma ball volume and surface recombination coefficient which are dependent on the reactor pressure. Dr. Dahimene said that until the reactor pressure was included in the linear growth rate calculation he felt that the model would not be a good predictor of growth rates. Dr. Dahimene offered to take another look at the model once the reactor pressure has been integrated into the model. (IBIS has since included reactor pressure as a variable. The results from this change will be shown in the first quarter 1994 report.)

Dr. Dahimene asked to run a few scenarios to see how the growth rate predictions matched his experiences in diamond growth. After running a few test cases he stated that the model was fairly accurate, estimating linear growth rates to within 0.2 u/hr on low power systems.

Summary & Conclusions

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